

Theory of Fano-Kondo effect in quantum dot systems: temperature dependence of the Fano line shapes

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Abstract

The Fano-Kondo effect in zero-bias conductance is studied based on a theoretical model for the T-shaped quantum dot by the finite temperature density matrix renormalization group method. The modification of the two Fano line shapes at much higher temperatures than the Kondo temperature is also investigated by the effective Fano parameter estimated as a fitting parameter.

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Conductance through quantum dots (QDs) as a function of gate voltage generally shows asymmetric peak structures due to the Fano effect. This structure is characterized by the Fano asymmetric parameter q . Concerning the theories of the T-shaped QD under the zero-bias condition, the Fano-Kondo effect studied so far has been limited to the $q = 0$ case[1,2,3], where conductance has dip structures at high temperatures and shows the anti-Kondo resonance at low temperatures.

To consider the finite- q case of the T-shaped QD, we introduce a simple tight-binding model[4] which is a one-dimensional Anderson model with an additional gate voltage ϵ_0 applied to the 0-th site.

$$\begin{aligned}
 H = & - \sum_{i\sigma} t_{i,i+1} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.}) \\
 & + \epsilon_0 \sum_{\sigma} c_{0\sigma}^\dagger c_{0\sigma} - v_d \sum_{\sigma} (d_{\sigma}^\dagger c_{0\sigma} + \text{h.c.}) \\
 & + \epsilon_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + U_d d_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow},
 \end{aligned} \tag{1}$$

$$t_{i,i+1} := \begin{cases} v_0, & \text{when } i = 0 \text{ or } -1, \\ t = 1, & \text{others,} \end{cases} \tag{2}$$

where QD has a single level, ϵ_d , and an on-site Coulomb interaction, U_d . It is important for this model that the Fano parameter is changed by the additional gate voltage: $q = \epsilon_0/\Delta_0 = \epsilon_0 t/2v_0^2$. Actually, zero-bias conductance g normalized by $2e^2/h$ is given by this parameter q and the local Green's function at the QD, $G_d(\omega)$. The local Green's function can be obtained by the finite temperature density matrix renormalization group (FT-DMRG) method after a numerical analytic continuation either by the maximum entropy method (MEM) or the Padé approximation. The results are characterized by two Fano asymmetric peaks at high temperatures and by the Fano-Kondo plateau inside a Fano peak at low temperatures. For further details, see ref. [4].

Strictly speaking, the Kondo temperature depends on the gate voltage, which can be written around the symmetric case: $T_K(\epsilon_d) \simeq \sqrt{\Delta_d U_d/2} \exp(\pi \epsilon_d (\epsilon_d + U_d)/(2\Delta_d U_d))$, where $\Delta_d = v_d^2/\Delta_0(1 + q^2)$. When the QD is doubly occupied and empty, the lowest characteristic temperature is the minimum of U_d and $\pi\Delta_d$.

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This characteristic temperature is smoothly connected to the Kondo temperature around the symmetric case[5]. Especially, two Fano peaks are modified at temperatures $T < \min(U_d, \pi\Delta_d)$, which is much larger than $T_K(-U_d/2)$.

In this paper, we study the modification of the Fano shape at the intermediate temperatures. We also compare the numerical results with the conductance obtained by the Zubarev's approximation, which is valid at high temperatures. One can see the difference between the numerical results and the Zubarev's approximation in Fig. 1(a). The difference becomes smaller when a local magnetic field is applied on QD to suppress the Kondo effect as shown in Fig. 1(b). Moreover, these results are very close to the non-interacting results. This fact means that the "one body level" picture is good if large Zeeman splitting is applied. In other words, the left (right) part of the right (left) peak in Fig. 1(a) is modified due to the many body effects which are described by beyond the Zubarev's approximation.

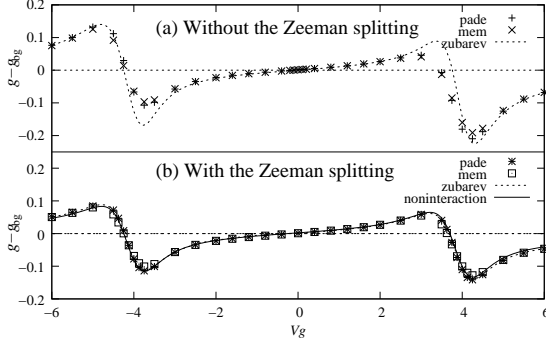


Fig. 1. (a) Conductance in a well separated case: $T/t = 0.2, q = -0.8, \Delta_0/t = 1, \Delta_d/t = 0.15 (v_d = 0.5)$ and $U_d/t = 8$. g_{bg} is a background current. (b) Conductance under a large Zeeman splitting $\Delta\epsilon_d = 4$ for $U_d = 4$. Other parameters are the same as those of (a). The line and the points are very close to the one of the non-interacting results with $\Delta\epsilon_d = 8, U_d = 0$.

To determine the modification of two Fano line-shapes quantitatively, we estimate the effective Fano asymmetric parameter q_T at a given temperature as a fitted parameter. In order to fit the shape of the Fano peaks, there are several possible ways as used in experimental analyses [6]. The simplest way may be to fit with the function,

$$g(V_g) = g_{bg} + g_a \frac{(e(V_g) + q_T)^2}{e(V_g)^2 + 1}, \quad (3)$$

$$e(V_g) = \frac{V_g - \Delta V_g}{\Delta_d T}, \quad (4)$$

with five fitting parameters $g_{bg}, g_a, q_T, \Delta V_g$ and $\Delta_d T$. In order to fit two Fano structures, we separate them

into two ranges: $-6 < V_g < -2$ and $2 < V_g < 6$ and fit the data in each range with the five parameters.

We plot the temperature dependence of q_T in Fig. 2 with several lines by changing the Zeeman splitting energy $\Delta\epsilon_d$. The difference of q_T between left and right Fano structures disappears when strong Zeeman splitting is applied. Especially, the difference between the data in $\Delta\epsilon_d = 0$ case becomes larger with decreasing temperature. Finally at zero temperature, the asymptotic behavior of q_T is expected to go toward 0 and $-\infty$ because the Fano asymmetric peaks at the high-temperature regime become a peak ($|q_T| \rightarrow \infty$) or a dip ($q_T \rightarrow 0$) in the low-temperature regime. In this sense, the temperature dependence of the estimated Fano parameter q_T can be regarded as a precursor of the Fano-Kondo effect for a finite q case. From the realistic viewpoint, it is important that this many-body effect is observable at relatively high temperatures $T/\pi\Delta_d \sim 1$ which is larger than the lowest Kondo temperature at the plateau.

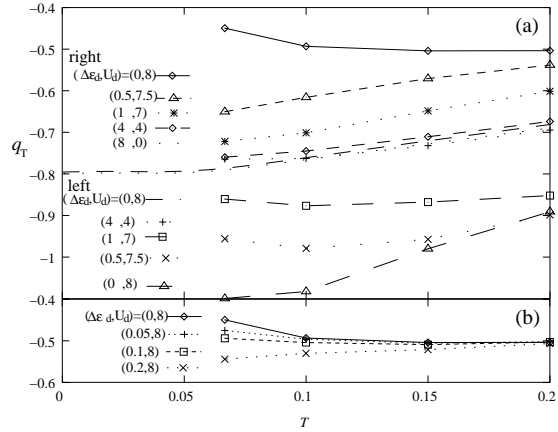


Fig. 2. Fitted results of q_T as a function of temperature. The fixed range, $-6 \leq V_g \leq -2$, is used for the fitting for the left Fano structure ($2 \leq V_g \leq 6$ for the right). The data are obtained for the results of $q = -0.8, \Delta_0 = 1, \Delta_d = 0.15$ with varying $\Delta\epsilon_d$ and U_d .

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